



Model-Based Gun Propellant Formulations

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FORWARD

The Model-Based Gun Propellant formulations Final Report is a report which describes in detail the results of the SERDP Pollution Prevention Project #1115 "Green Energetic" and meets the final reporting requirements. This project was sponsored by the Strategic Environmental Research and Development Program, Arlington, VA 22204. Questions may be directed to Randall J. Cramer, Naval Surface Warfare Center, Indian Head Division, Indian Head MD 20640.

MODEL-BASED GUN PROPELLANT FORMULATIONS

INTRODUCTION

New energetic materials, new explosives, and propellant formulations have traditionally been developed through the following long-standing process. Chemical structures of new energetic compounds are identified and the discovery of suitable synthesis procedures for these new candidates becomes the target of initial research efforts. These synthesis procedures once identified, are repeated and further optimized until the process using laboratory methods is efficient enough to produce small quantities of material. Exploratory development programs are then initiated to formulate, evaluate and further scale-up the synthesis of these materials. These steps are reproduced and repeated to further provide enough material for assessing the new composition's performance, sensitivity, safety and vulnerability properties. Once the properties of the composition have been cataloged, the data is made available to program managers and weapon systems designers, and the composition is offered as a potential candidate for incorporation into their programs. Based on the information provided from the basic research and exploratory development efforts, the customer or user may then select a composition that either offers some degree of improvement in their respective programs or which help them meet some predefined performance requirements. Once again, steps can then be undertaken to scale-up and make even larger quantities of material for use in advanced testing and evaluation.

Although a number of useful materials and detailed databases have been developed through this process, there are three major drawbacks that need to be addressed to improve the business of introducing new materials into Navy weapons programs. One serious deficiency is this process is driven by materials development rather than by customer's or user's requirements. Granted, a new material is targeted with some notion of a final application and performance requirement in mind, but for the most part, the material is developed and then evaluated, and the results are presented to a number of program managers as a potential candidate to meet their particular needs. A second drawback to be noted is this process requires repeating the synthesis, formulation, and mixing of the material for each stage of the new material's development and for each time a test is to be conducted. All of these steps produce waste. Although a significant amount of essential data is obtained from the testing and analysis of these products, none of the product that is produced under this process is dedicated to the mission for which the material had originally been designed; and that would be to deliver a weapon to its target. From an environmental impact standpoint, all of these products produced during the development of the material must be considered as waste. In addition, it can be seen, from a pollution prevention standpoint, that environmental impact and environmental analysis is either absent all together from this process, or environmental cost analysis is performed after the material has gone into production. This means environmental cost analysis is conducted after the fact, which is not consistent with the pollution prevention mission.

This report describes a new process and a new development tool that has been specifically designed to introduce pollution prevention concepts into energetic materials development.¹ This process intends to improve upon the three problem areas cited above. Energetic materials development is driven by the user's requirements rather than by the availability of a new material; the number of the scale-up experiments, and, hence, the resulting waste generated from these small scale mixes and tests are eliminated or reduced; and, most important, environmental cost estimations using models and predictive technology can be made prior to entering development. This model-based approach provides technologists with the ability to perform energetic materials formulation and obtain developmental cost information using a systematic automated design. To accomplish this for energetic materials, an integrated method built upon proven models, well-defined components, established data correlations and databases were developed. This method is referred to in this paper as the Model-Based Gun Propellant Formulations approach.

GENERAL MODEL ARCHITECTURE

The objective of the first phase of this program was to design a model-based architecture which would, based upon a given set of performance and environmental constraints, identify energetic compositions and their respective environmental and non-environmental development costs. The structure of this architecture was to be built upon existing predictive codes, models and databases. Once the general design of this tool was determined, demonstration of its utility was to be performed using a known set user's requirements.

The available models, codes and databases needed to perform the first phase of this development were identified by the experts in the field of energetic materials research and development, weapon system performance, materials processing and demilitarization through the participation in the Model-Based Formulations Workshop.¹ A number of conclusions were obtained as a result of this workshop. Since building a working model which encompasses all the different types of energetic materials compositions is an overwhelming task, the group decided to better define the initial scope of the model. The working group agreed to focus the initial phase of this effort upon gun propellant technology with the allowance for the future expansion of the architecture to include explosives, rocket propellants and pyrotechnics. With this in mind, an overall approach containing the elements for modeling performance, sensitivity, stability, processing, and environmental cost of gun propellant development was constructed. The resulting general architecture and the flow diagram is given in Figure 1.^{2,3}

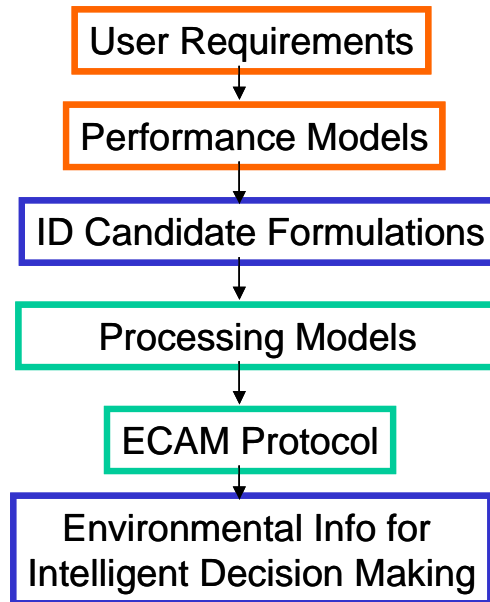


Figure 1. Flow Diagram For The Model-Based Formulations Architecture

This model-based approach is unique in that it begins with the user requirements as inputs into the overall modeling structure. This step brings user requirements and environmental constraints into the front end of the modeling process. This procedure also assists the user in identifying or evaluating alternative materials and reducing the use of hazardous material in new formulations. This pollution prevention step becomes vital, as it is part of the architecture's input information required for operation of the entire model. Further examples of both the environmental and performance inputs are given in Table I.

Table I. Model-Based Gun Propellant Formulations User Inputs

<u>Performance Requirements:</u>	<u>Environmental Constraints:</u>
✱ Projectile Weight	◆ Toxic Chemical Limitations (e.g., heavy metals, carcinogens, etc.)
✱ Velocity	◆ HAZMAT Handling and Waste Requirements
✱ Breech Pressure	◆ TRI Reduction Requirements
✱ Allowable Flame Temperature	◆ The Use of Pollution Prevention Technologies
✱ Firing Scenarios	◆ Reduction in the Use of Non Recyclable Resources
✱ Chamber Volume	◆ Any Disposal Restrictions
✱ Flash Limitations	
✱ Cost	
✱ Desired Energy	
✱ IM Requirements	

These inputs provide the basis for determining a formulation or a series of formulations that meet the user's requirements. Not all of the inputs listed are needed to perform the desired analysis, although just as in any analysis, the more information that is provided up-front, the more specific will be the final output and results.

The first major step in this design is the modeling of a formulation that meets the requirements set out by the input information. This step is symbolized by the "Performance Model" and the "Identification of Candidate Formulations" boxes in Figure 1. There are already a number of existing sophisticated ballistic and thermodynamic codes available for use to model gun propellant formulations. The significant amount of existing data and a number of databases can be combined for modeling formulations based on ingredient compatibility, stability and vulnerability. These codes and databases can be integrated in such a fashion as to create a "virtual gun system". From a chemical and thermodynamic description, each propellant is then characterized in the weapon without ever having been placed in the gun chamber. The environmental cost saving that result from modeling formulations and eliminating the synthesis, processing, packaging, transportation, and testing of each and every new formulation is, of course, substantial.⁴

The second step in the model is to obtain the environmental cost information based a simulation of the processing of the candidate formulations. A review of modeling and the available process simulations for continuous and batch solvent and solventless processes was performed.⁵ This review noted that models which provide the relationships between the macroscopic process variables are not available. Therefore, a simulation that relates the activities, time and costs associated with processing the gun propellant composition from raw materials to cut propellant grain was developed under this phase of the program. Since this simulation is activities based, the design was amenable to the inclusion of the costs associated with both the environmental and nonenvironmental (materials cost, labor, etc.) activities. The simulation design is such that it can also be used to identify process-specific resource requirements, types of waste streams and their content.

The environmental and other costs associated with processing of the material are determined based on the process simulation through the use of the Environmental Cost Analysis Method (ECAMSM).⁶ This method was developed by Concurrent Technologies Corporation (CTC) through the National Defense Center for Environmental Excellence, in cooperation with Coopers & Lybrand, L.L.P. Up to this time, ECAMSM has been applied to existing facilities to obtain a consistent means of quantifying and evaluating environmental costs and benefits based on activity based costing. ECAMSM has been applied at five DOD locations in which environmentally preferred technologies have already been fielded or are being evaluated for future use. Each of these technologies is designed to eliminate or reduce potentially adverse environmental impacts, while simultaneously cutting costs and maintaining or improving product quality. In this modeling approach, environmental financial information based on a simulated process was obtained by applying ECAMSM to a process simulation. In the model-based gun propellant formulations design, the process simulation acts as the

facility, and the unique application of ECAMSM in this model provides environmental and other economic information related to processing the candidate formulation.

In addition, the cost associated with demilitarization was modeled through the use of a Resource Recovery and Reuse (R³) Demilitarization Algorithm developed under this program. This algorithm estimates the cost of demilitarization, recovery of key ingredients and treatment/disposal of waste using a special key feature that expressly bases its calculations upon the implementation of new technology for R³. The final cost analysis provides the balance of the money gained through recovering and recycling the materials with the cost incurred through disposal.

The model-based formulations output provides a breakdown of the environmental costs associated with the processing of a gun propellant formulation that meets the user environmental and performance inputs. A variety of means for presenting and comparing a candidate formulation's environmental costs are available as outputs. For example, environmental costs can be expressed as a percent of total cost, and the environmental costs of different candidate formulations can be compared and contrasted. A breakdown of the environmental costs can also be made in a number of ways suitable to meet the user's needs in a decision making process.

Finally, it was also the general opinion of the workshop that it would not be practical to set out to write a fully automated computer code. Rather the initial stages of development should focus on the demonstration and utility of the models to be used. Therefore, a degree of manual intervention will be necessary to perform the first demonstration of the architecture and the environmental analysis. One must keep in mind, of course, a long-term goal is to wrap the codes and databases in such a fashion that the system is completely automated and available for use through an Internet web site. The architecture developed here will be the first step in achieving this goal, and will allow ready substitution and continual improvement as the new methods are developed and as the various predictive codes become more sophisticated.

PERFORMANCE ALGORITHM

The performance algorithm is the set of codes and databases that can be integrated in such a way as to provide a candidate formulation based upon the environmental and performance requirements input.⁷ The following sequence was developed to provide a basis for the performance algorithm:

Step 1: The model will "choose" a formulation based on the user's inputs from a library or a propellant database composed of known and/or new propellant formulations.

Step 2: Those propellants containing known environmentally unacceptable materials (lead, dinitrotoluene, etc.), or which do not otherwise meet up-front environmental constraints will be screened out of the performance testing process. The screening is not only based on the

ingredients themselves, but also the manufacturing processes involved in creating the material.

Step 3: Each propellant must be described by a suite of measurable physical parameters in order to be acceptable to the Interior Ballistics, IB computer programs. Required values include isochoric flame temperature, density, internal chemical energy, and others depending on which computer code is finally used for performance modeling. Several programs are available to estimate these parameters (except for density and burning rate) from the initial chemical description. These programs include CHEETAH⁸, BLAKE⁹, and the NASA-Lewis Code^{10, 11}. Propellant density and burning rates must be physically measured or estimated from other sources. A series of curves for burning rate coefficient verses flame temperature (the exponent would be a constant for each class of propellant) for different classes of gun propellants using existing data were generated. Through the use of these curves, an appropriate burning rate equation for each candidate propellant can be selected.

Step 4: Given a gun system model and the thermodynamic properties of each propellant, an estimate can be made of how much energetic material can be placed in the gun chamber. A calculation can then be made to determine if enough kinetic energy can be transferred to the projectile in order to meet the exit velocity requirements. By assuming that the highest allowable pressure is continuously maintained by propellant combustion (until the charge is exhausted), an estimate of maximum achievable projectile exit velocity can be calculated. If this velocity does not meet or exceed user requirements, then the propellant will not be a candidate for further testing. The computer code used to estimate this maximum is CONPRESS.¹²

Step 5: An IB performance program is used to find possible propellant grain geometries that will satisfy user gun system requirements. The IB calculations can determine if one or more propellant grain designs can be used as charges in the gun system to can meet requirements for muzzle energy and complete charge burnout within maximum pressure limitations. A first-pass IB program is IBHVG2. Starting with the most progressive geometries (19-perf, 7-perf) grain configurations are sequentially evaluated to provide propellant configurations, which satisfy Step 4. These geometries are tested, as far down as single-perf to determine how much grain design flexibility is possible for each propellant type.

Step 6: This step tests for charge burnout (i.e., muzzle blast and flash). The grain geometry meeting minimum energy requirements at maximum charge weights must still show complete burnout when used at lower

loading densities. The same IB programs used for calculating acceptable propellant grain geometries are also used here.

Step 7: Other conditions included as inputs which have not been addressed at this point of the modeling process are now considered. Cost, manufacturing limitations, burning temperature (a major factor in gun tube life expectancy), grain size, or any number of user-defined stipulations may preclude propellants from final consideration. More likely, the list of remaining propellants will be ranked according to importance of these additional factors.

By prioritizing the property to be maximized or minimized and setting any limits on other properties (e.g. highest possible impetus while keeping flame temperature below a certain value) optimization routines on the models as shown above can be used to determine the formulation. If the desired properties are not achievable with those ingredients, different ingredients may be selected and the process repeated until the best fit is obtained.

Predictive methods for assessing gun propellant vulnerability were developed and included in the architecture. A database was created for the various classes of gun propellants, and empirical correlations based on ingredients were established for a gun propellant's critical diameter, failure diameter and thermal decomposition. This database can be used to determine whether a formulation will pass or fail shaped charge jet impact and cook-off.

Of significant interest are the tables that relate the critical diameter of the six classes of propellants (single base, double base, triple base, nitramine, nitramine inert TPE, nitramine energetic TPE) to shock initiation response. In the case where the propellant web thickness is twice the size of the critical diameter, a violent response would be exhibited when impact by a shaped charge jet. This database is then used to relate the formulation and its critical diameter to vulnerability response.

Two approaches are possible for predicting the acceptability of the long-term storage stability. One approach uses the wealth of stability data available to generate shelf life prediction templates for the variety of stabilizers used for each class of gun propellant compositions. A second approach uses rate expressions derived from measured thermal decomposition rates as the foundation for the prediction templates. The first method would provide results based strictly upon stabilizer depletion rates, and the second method would depend both upon the binder system and stabilizer used in the composition.

There is much stabilizer depletion rate data available for the limited number of stabilizers of concern. This data needs to be gathered from the existing literature and assembled for use in the model. The degradation of propellant can be modeled if kinetic data are available, and the activation energies, rate constants and other rate dependence

factors are known. This information is frequently not even available for existing formulations.

PROCESS SIMULATION

Once a formulation has been selected through the use of the above performance algorithm, processing of the formulation is then simulated using a process simulation. This simulation was developed specifically to provide a tool for the calculation of the environmental costs associated with the processing of the candidate formulation.¹³ The simulation includes solvent based and solventless processes for both continuous and batch process facility. This module was designed to take discrete information from each activity of the process and calculate the utilization and operating times. This in turn calculates cost and energy requirements. A chart which shows the process flow diagram of the simulation broken down into three parts; process set-up and preparation, production activities, and finishing shutdown and cleanup are shown below.

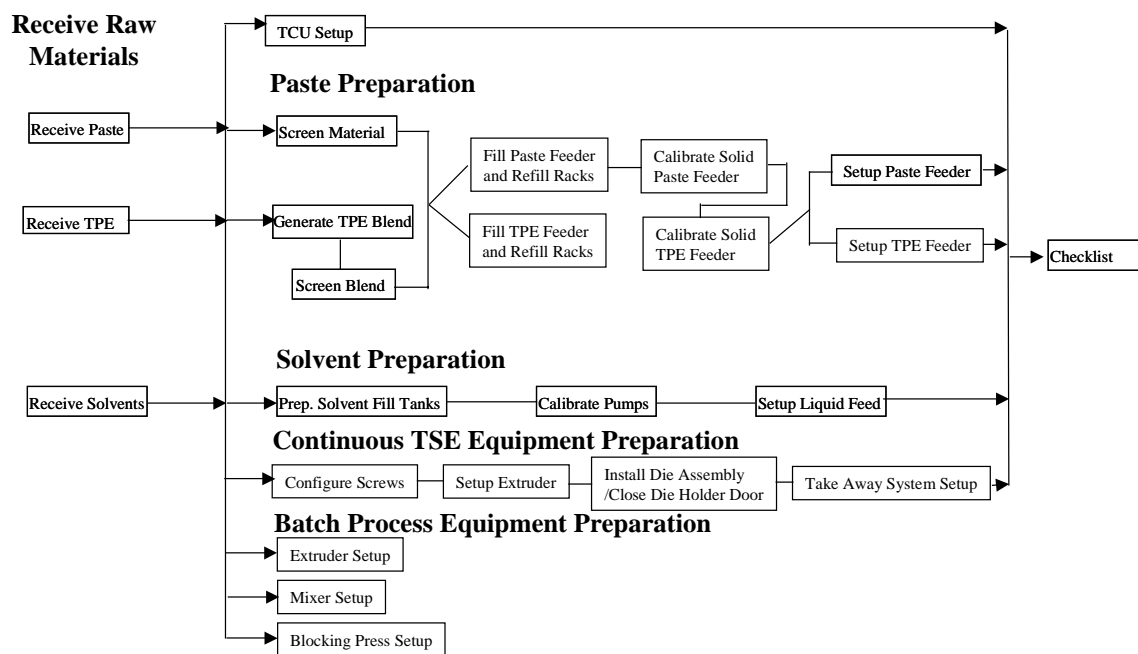


Figure 2. Continuous and Batch, Solvent and Solventless Process Preparation Activities

The process simulation information was compiled conveniently into Excel spreadsheets. This allows easy modification or adjustment of the input information so the model can be used to simulate different facilities and to switch from continuous to batch processes if one desires. EXTEND software was used to develop a graphical representation of the process and to calculate the required outputs based on the set of given inputs.

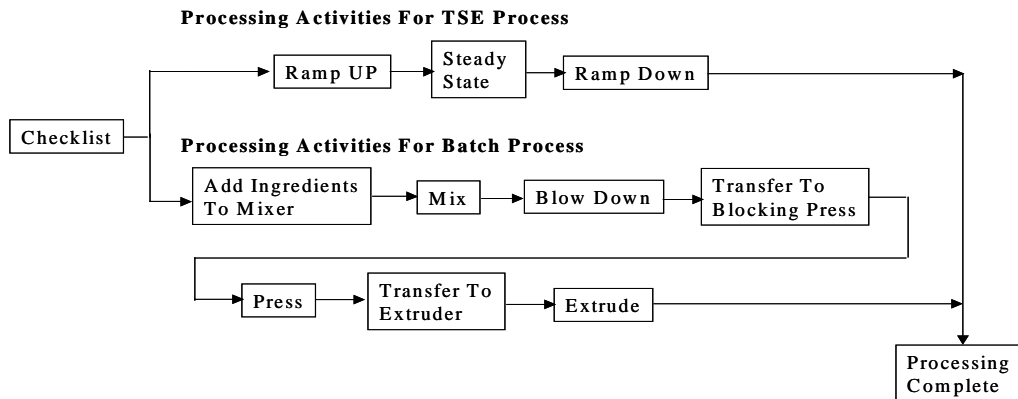


Figure 3. Twin Screw Extruder and Batch Processing Activities

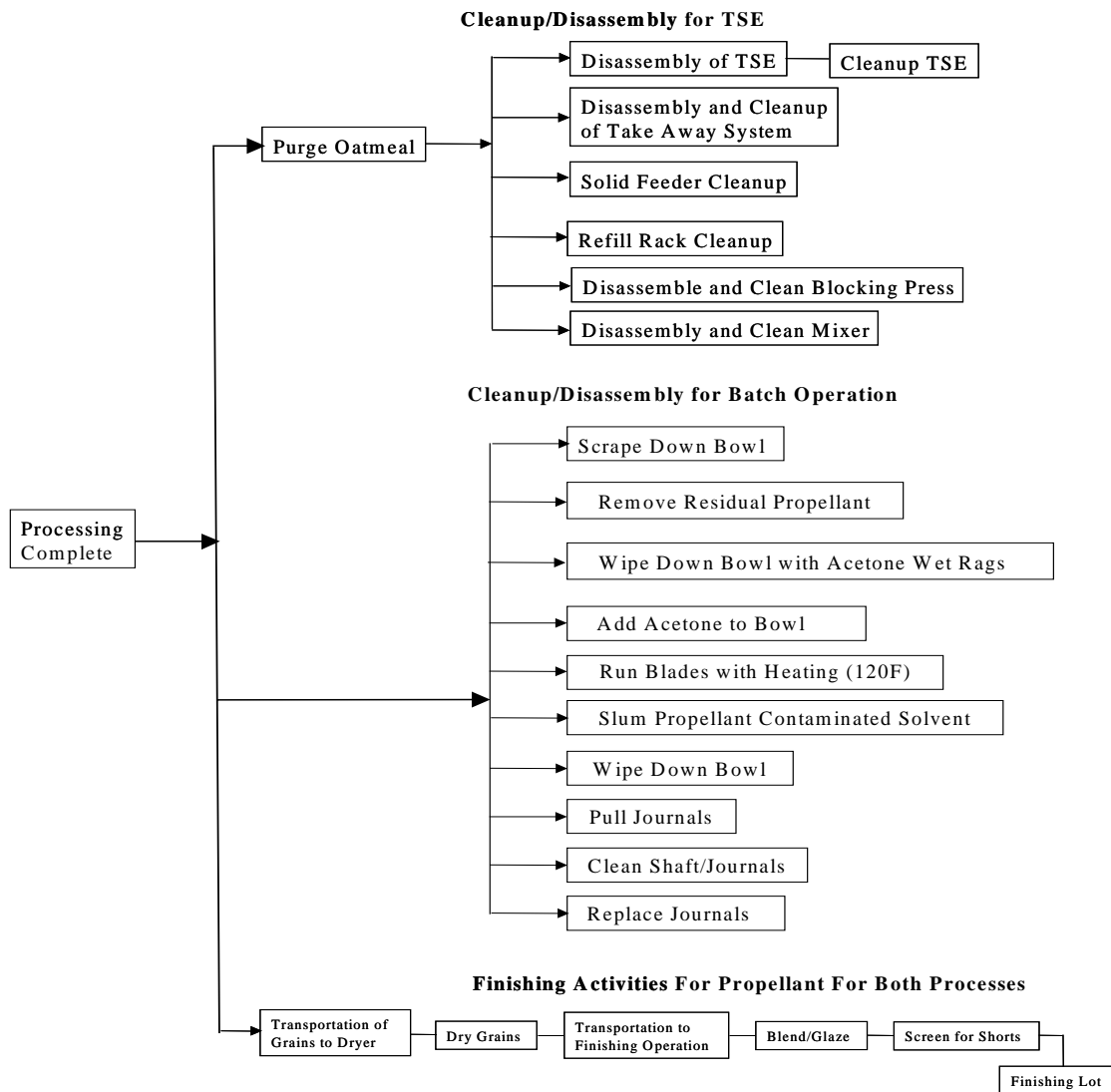


Figure 4. Cleanup/Disassembly And Finishing Activities

ENVIRONMENTAL COST ANALYSIS METHOD

ECAMSM provides a standard approach for handling direct and indirect costs associated with processing of the propellant. Environmental costs are evaluated and quantified using activity-based costing principles. A general depiction of the ECAMSM process is shown in Figure 5.

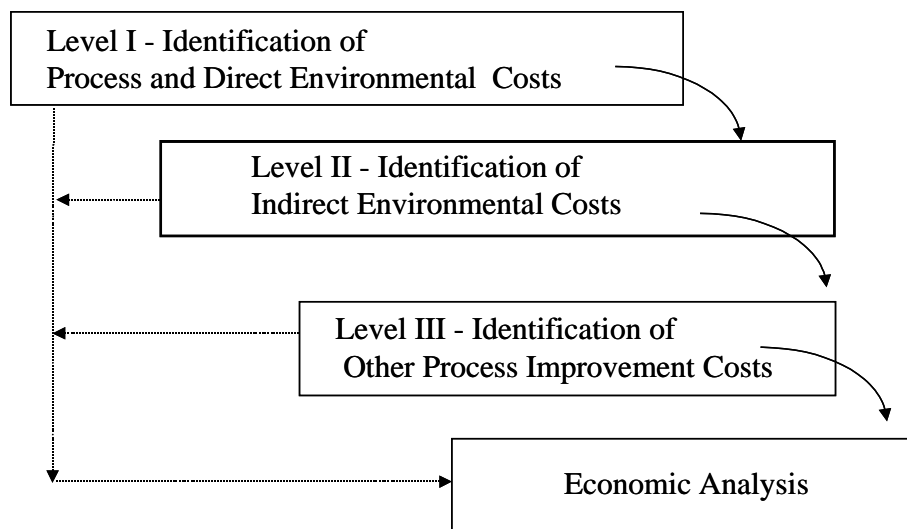


Figure 5. *The Environmental Cost Analysis Methods*

In the process simulation, the activities of the process were also categorized by the type of the environmental activity. This allows one to view the contribution of environmental cost to the total costs of the process, as well as, a breakdown of the types of environmental costs. The categories devised for this simulation were as follows:

1. *Documentation* - Defined as all documentation of the process required for environmental reasons, including but not limited to documentation of all appropriate information for the compliance documentation of permits, material tracking, etc.
2. *Permitting* - Defined as all activities required to obtain and maintain existing permits, not including documentation to prove compliance (which is covered under documentation above).
3. *Pollution Prevention* - Defined as normal activities currently completed so as to limit unnecessary release of hazardous materials.
4. *Air Emissions* - Defined as the amount and cost of VOC air emissions and their abatement. This also includes abatement equipment upkeep.

5. *Solid Waste Material* - Defined as the amount of solid waste generated. This includes waste material and miscellaneous such as gloves, container etc. Also included here was the cost of the amount of scrap material generated. The cost of the amount of scrap material generated is iteratively calculated as it is based on the final cost of the material production. This method was used to accurately represent the fact that the added value (production process) has been put into the material and that value is lost in the scrap material.
6. *Solvent Waste Material* - Defined as the amount of waste material saturated or contaminated with solvent. These items include solvent laden gloves, lines, containers etc.

Energy consumption and costs were determined through the use of commercially available energy modeling software.¹⁴ There are a number of energy analysis software packages available on the market today. These packages can estimate a facility's energy use and provide output showing annual energy consumption on a monthly basis. This analysis takes into account variations in weather and is easy to modify so that "what if" type runs can be performed with minimal effort.

RESOURCE RECOVERY RECYCLE AND REUSE ALGORITHM

A module was developed to assess the cost for demilitarization of the propellant charge.¹⁵ Destructive technologies like open burning/open detonation (OB/OD) result in end products which contribute to air, water, and soil pollution. Also, these demil costs are usually estimated using a flat rate per pound, and estimations of this sort do not really add much value in this type of analysis and evaluation. Therefore, a new approach for estimation of demil costs was developed. An alternative algorithm was developed which includes materials reclamation in addition to materials demil and disposal. Consistent with the current DOD emphasis on the reclamation and reprocessing of energetic materials uses, current or emerging resource recovery and reuse (R3) technologies is included in this module.

This model captures and predicts the economic and environmental costs associated with demilitarization activities. The flow chart for this module is given in Figure 6. The analysis begins with the formulation ingredients and the total amount of propellant produced. These inputs are obtained from the above candidate formulation and process simulation. The analysis then proceeds to provide an output balance determined by difference of reclamation dollars and the total demilitarization process and disposal costs. This module has also been specifically designed to obtain estimated cost information on new technologies as they are developed. This also provides a route for the evaluation of the payoffs and drawbacks of new reclamation technologies that may otherwise remain neglected.

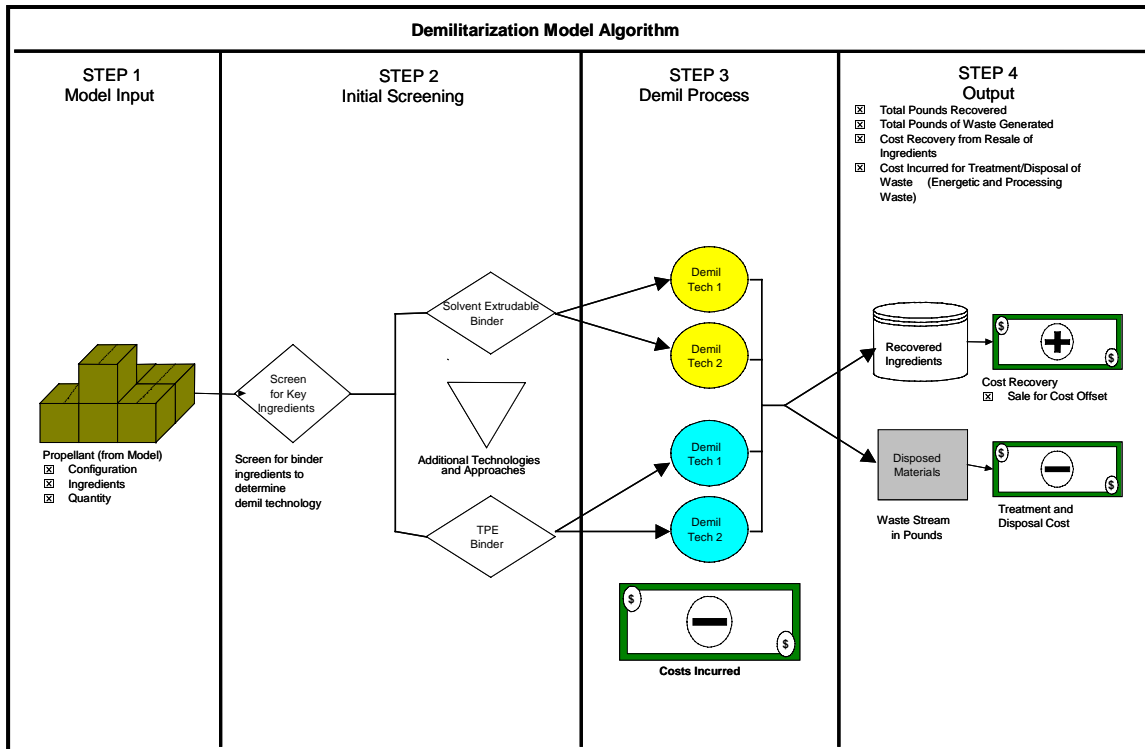


Figure 6. Resource Recovery Reuse Demilitarization Algorithm Flowchart

DEMONSTRATION OF THE MODEL-BASED APPROACH

The feasibility of this architecture and a demonstration of the types of outputs and cost information one may obtain using this modeling approach was performed using a simple set of inputs.¹⁶ Using 5-inch 54-caliber gun system requirements and the environmental constraint the formulation be lead free, two candidate gun propellant formulations were generated from the performance algorithm. These formulations differ in that one candidate is a solvent processed nitramine propellant and the second candidate is a solventless processed nitramine propellant with an energetic thermoplastic elastomer binder system. These two formulations provide the basis for illustrating the use of the newly developed process simulation and the application of the ECAM analysis in providing environmental cost information, and for making a direct comparison of the predicted costs of two very different formulations and processes.

Performance Algorithm

As a test system, the Navy 5-inch 54-caliber gun was chosen to be the vehicle for exercising the performance algorithm. User-supplied guidelines included a maximum pressure limitation of 65 kpsi (448 MPa) and a minimum muzzle energy of 18MJ with a 110-lb (49.9-kg) projectile. From the kinetic energy formula ($KE = \frac{1}{2} MV^2$) it can be determined that projectile velocity needs to be at least 848 m/s to meet the requirement.

A general description of the weapon specifies a chamber volume of approximately 0.0151 cubic meters (919 cubic inches) and projectile travel of 6.84 meters (269 inches).

For this demonstration, the performance algorithm proceeded as follows:

Step 1: Develop Database For Consideration

A mixture of old and new propellant formulations, from both Army and Navy sources, provided a well-rounded sample for the analysis. All propellants are real, in other words, no theoretical materials have been added to the study, although this could certainly be done in future tests. The standard Army propellants include: M1, M10, M26E1, M30A1, M31E1, and JA2; Navy propellants are NACO, EX99 (called LOVA in the reference noted in Table 2), HELP42, and BAMO/AMMO (abbreviated as BAMO in the rest of this report). For the purposes of this demonstration, an attempt was made to include the different classes (single-base, double-base, and triple-base) of propellants, along with some newer formulations not fitting neatly into such descriptions.

Step 2: Screen Based On Environmental Constraints

The propellant library used in this demonstration is given in Table II. A quick scan reveals that NACO contains lead carbonate – a known toxic substance and suspected carcinogen.¹⁷ For this reason, NACO was dropped from further analysis

Dinitrotoluene, (DNT is an ingredient of the Army M1 propellant. The International Chemical Safety Card (ICSC 0727)¹⁸ describes this substance as absorbable through human skin, and ingested through inhalation of fumes when it is heated. For humans it is an irritant to eyes and skin, and may cause effects on the central nervous system, cardiovascular system and blood. It is also extremely toxic to aquatic organisms. The environmental costs from DNT can be very high; as an example of the type of chemical ingredient to be avoided, mixtures with DNT (specifically M1) will be removed from the list of propellants under consideration.

Table II. Propellant Library

Propellant	Ingredients	Reference
M1	NC1315 DNT DBP DPA H2O ALC	Freedman ¹⁹ , p. 121
M10	NC1315 DPA KS H2O ALC	Freedman ¹⁹ , p. 121
M26E1	NC1315 NG EC H2O ALC C	Freedman ¹⁹ , p. 122
M30A1	NC1260 NG NQ EC KS ALC C	Freedman ¹⁹ , p. 122
M31E1	NC1260 NG NQ DBP NDPA KS ALC C	Freedman ¹⁹ , p. 122
NACO	NC1200 BS EC KS PB2CO4 H2O ALC	Freedman ¹⁹ , p. 122
JA2	NC1304 NG DEGDN AKAR2 MGO H2O C	Miller ²⁰
BAMO	RDX BAMO AMMO	Almeyda ²¹
HELP-42	HZTZ RDX NC1260 BDNPF BDNPA EC	Cramer ²²
EX-99	RDX NC1260 CAB BDNPF BDNPA EC	Cramer ²²

Step 3: Determine Modeling Information

The thermodynamic values needed for these compositions can be calculated using CHEETAH, BLAKE or the Nasa Lewis Code, and burning rates were obtained from published values or estimated from like materials.

Step 4: Test For Available Energy

IBHVG2 computations were used to evaluate the potential energy of each propellant in the gun system model. The purpose of this step is to quickly determine whether the charge could meet the minimum requirement of projectile exit velocity while keeping chamber pressure no higher than the user-defined maximum. The program artificially ties breech pressure to a given value (by converting the necessary amount of propellant to gas at each time step) until the charge is completely burned; then the gases are allowed to continue expanding (and accelerating the projectile) until maximum travel is accomplished. This process approximates what would be the perfect combination of propellant surface area and burning rate in order to transfer maximum energy to the projectile. CONPRESS does not require estimates for either grain geometry or burning rate; IBHVG2 requires either burning rate or grain geometry, although this is just a formality – both can be made to vary in order to complete the calculation.

Computed projectile exit velocities using IBHVG2 are listed in Table III for each of the remaining candidate propellants. The user-required velocity is 848 meter/second; each velocity in the table is compared to that value via a percentage of minimum requirements. All considered propellants except M31E1 attained over 100% of minimum and will be passed on to the next step in the study.

Table III. Constant-Pressure Calculations Of Exit Velocity

Propellant	Exit Velocity (m/s)	Comparison %
M10	867	102.2
M26E1	858	101.2
M30A1	886	104.5
M31E1	825	97.3
JA2	902	106.4
BAMO	914	107.8
HELP-42	879	103.7
EX-99	894	105.4

Step 5: Determine Propellant Grain Geometry

A parametric feature allows IBHVG2 to vary propellant grain dimensions to calculate the effect of each geometry on performance in the modeled gun system. By adjusting one grain measurement (in this case the web, or burn-through distance between grain perforations and between the outer grain surface and closest perforations) the program can compute entire ballistic cycles for a series of grain sizes and can find the maximum pressure and the expected projectile exit velocity for each situation. The results are summarized in Table IV -- each propellant is listed with the three grain types, their corresponding web sizes for 448 MPa maximum pressure, and the calculated projectile exit velocity in each situation.

Table IV. Summary Of Gun System Run Performance Calculations

Propellant	19-Perf	7-Perf	1-Perf
M10	844 m/s (2.56 mm)	841 m/s (2.76 mm)	807 m/s (3.82 mm)
M26E1	836 m/s (3.48 mm)	835 m/s (3.76 mm)	806 m/s (5.20 mm)
M30A1*	861 m/s (3.06 mm)	856 m/s (3.34 mm)	812 m/s (4.72 mm)
JA2*	875 m/s (4.42 mm)	867 m/s (4.91 mm)	812 m/s (7.20 mm)
BAMO*	881 m/s (3.13 mm)	877 m/s (3.47 mm)	859 m/s (5.06 mm)
HELP-42	807 m/s (0.883 mm)	813 m/s (0.980 mm)	836 m/s (1.375 mm)
EX-99*	845 m/s (2.29 mm)	858 m/s (2.52 mm)	845 m/s (3.57 mm)

Step 6: Burnout, (muzzle blast and flash)

There was no requirement for this run.

Step 7: Rank Propellants According To User Desirability

In this run, BAMO and Ex-99 are ranked as the most suitable propellant. M30A1 and JA2 both provided solutions with the multi-perforated grain types, but not with the single-perf geometry.

Process Simulation

Two compositions, Ex-99 solvent processed composition, and BAMO, a solventless processed composition, were the resulting top candidates from the above library of gun propellant formulations. These two compositions were then used to demonstrate the use of the process simulation in the model-based formulations architecture. Environmental costs for each formulation were determined, for example, for a 200-pound lot of each material with the materials cost shown in the Table V (provided as default values in the simulation).

Table V. *Material Cost Inputs for the Process Simulation*

Process	Materials	Costs
Solvent	Solvent A (Ethanol)	\$1.50 / lb.
	Solvent B (Ethyl Acetate)	\$1.50 / lb.
	Paste	\$50.00 / lb.
Solventless TPE	RDX	\$8.53 / lb.
	TPE Blend	\$50.00 / lb.

The output, of course, can be configured in a number of different fashions, but this example shows a comparison of the labor, material and environmental costs for both formulations, as well, as a breakdown of the costs associated with the various environmental categories.

Table VI. *Cost Information Output File*

\$ Non-Environmental	Solvent	TPE
Labor:	\$7,669.66	\$13,453.24
Materials:	\$11,469.13	\$3,915.74
\$ Environmental		
Documentation:	\$766.97	\$230.09
Permitting:	\$383.48	\$0.00
Polution Prevention:	\$236.98	\$0.00
Air Emissions:	\$40.82	\$0.00
Solid Waste:	\$3,730.67	\$482.20
Liquid Waste:	\$50.00	\$0.00
Total \$ Environmental:	\$5,208.93	\$712.29
al \$ Non- Environmental:	\$19,138.79	\$17,368.98
Total Costs:	\$24,347.72	\$18,081.27

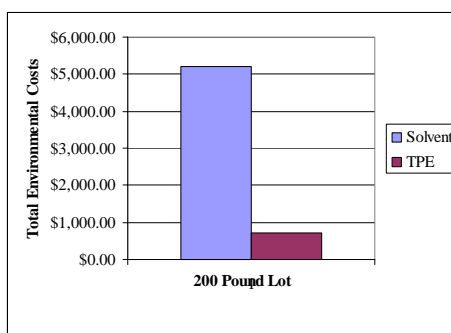


Figure 7. Environmental Cost Comparison for The Two Propellants

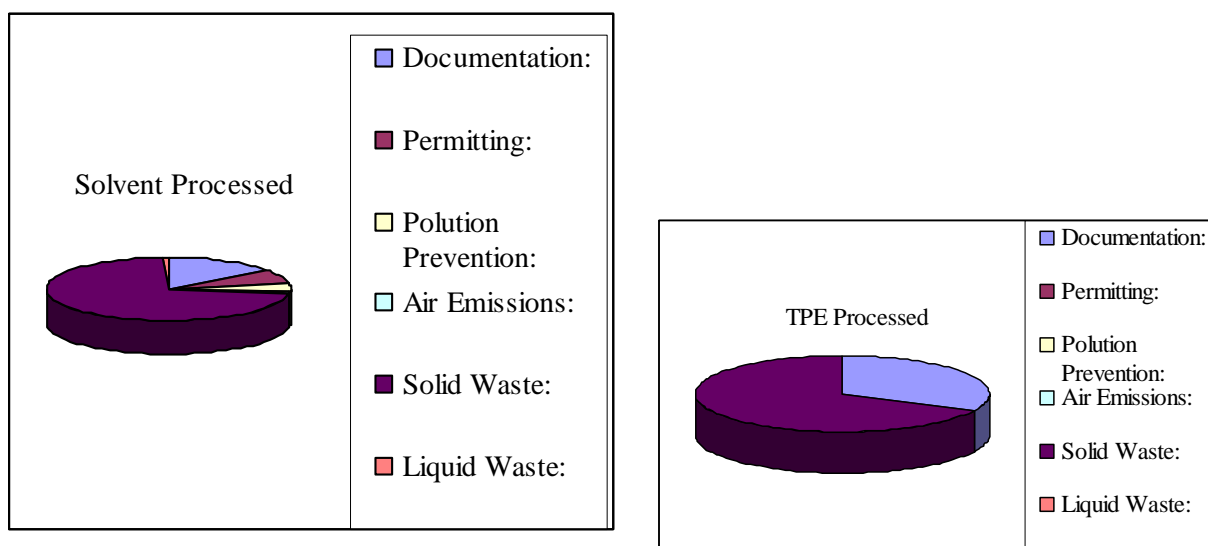


Figure 8. Environmental Cost Analysis Output File

Environmental Cost Analysis Method

As mentioned earlier, ECAMSM consists of four general steps. The first two steps provide environmental cost information based on process activities, and the final two steps are useful for obtaining additional economic information to allow an assessment of the total financial investment. ECAMSM uses three performance measures for evaluation of the investment: payback period, net present value (NPV) and internal rate of return (IRR). The payback period is the time required to recover 100% of the capital investment with the predicted cost benefits. The NPV is the value in today's dollars of the discounted future savings applied against the initial capital investment. A positive NPV indicates a profitable project. The IRR is the discount rate at which NPV is equal to zero.

The commercially available software P2/FINANCE was used to calculate these indicators.²³ This software allows representation of different investment options under consideration and use of the financial indicators to assess the investments profitability.

This software can be readily integrated into the current model-based formulations architecture.

The financial analysis using P2/FINANCE was performed for processing the two candidate formulations in a twin-screw extruder. The pilot-plant process simulation provides the operating cost for both compositions. Using the operating costs for the solvent processed propellant formulations as the baseline, the financial indicators were then determined for the alternative solventless candidate.

For example, the set of these costs for the annual production of 100,000 pounds of propellant for both the solventless and solvent processed candidates are shown in Table VII. These operating costs were then used as inputs into the financial analysis model. The resulting environmental indicators were determined for a twin-screw facility that has an initial investment cost of \$20,000,000. To simplify the demonstration, a 10% discount rate and zero inflation and zero income tax rate (although other values can be used if desired) were also used as inputs. The financial analysis of the investment for the solventless processed propellant compared to the solvent processed propellant is shown in Table VIII.

Table VII. Annual Operating Costs for Candidate Propellants (100,000lbs/yr)

Annual Operating Costs	Cost Solventless Processed (\$)	Cost Solvent Processed (\$)
Materials	1,894,485	5,677,714
Utilities	553,850	44,510
Labor	6,726,620	3,834,830
Waste Management	241,100	1,890,335
Regulatory Compliance	115,045	714,125

Table VIII. Profitability Analysis

Years	NPV (\$)	IRR (%)	Payback Period
0 – 5	<10,027,420>	-12.0	
0 –10	<3,835,232>	5.3	
0 -15	10,109	10.0	
			15 years

This analysis shows the annual production of 100,000 pounds of the solventless propellant in a new \$20M facility will experience a fifteen year payback in cost savings over the production of the solvent processed candidate using current facilities and process steps. It must be cautioned that the dollar amounts presented here were derived from default values and should be considered as examples only.

Resource Recovery Recycle and Reuse Algorithm

Resulting demil and life-cycle costs were determined in this model using the R³ Demil Algorithm. For the purposes of this analysis, the full-scale plant with a capacity of recovering 4,000 pounds of RDX per day was considered. The five scenarios presented are quantity variations of 100,000-pound increments, starting at 100,000 pounds. The cost estimates are based on 2,000 hours in one year (10-hour shifts, 200 days per year). IHTR 2036 presents the labor and material charges together at \$2.50 per pound.²⁴ An additional cost for recrystallization and fluid energy milling of \$6.00 per pound is added to these direct production costs. This subtotal cost of \$8.50 per pound is adjusted from fiscal year 1997 to 1999 dollars, totaling \$8.53 per pound for the cost of demilitarization.

The baseline cost of virgin RDX material used for this cost and environmental analysis was \$13.06 per pound. It is assumed that the market for reclaimed RDX will support 50% of the baseline RDX cost. Thus, the resale of RDX results in \$6.53. The total net cost of the reclamation of RDX is \$2.00 per pound (Table IX).

Table IX. Demilitarization Costs for EX-99 Propellant

Pounds of Energetic per Year	100,000	200,000	300,000	400,000	500,000
Labor & Material (\$/lb)	2.50	2.50	2.50	2.50	2.50
Additional Cost of Recrystallation / Fluid Energy Milling (\$/lb)	6.00	6.00	6.00	6.00	6.00
Subtotal Direct Production	8.50	8.50	8.50	8.50	8.50
Adjust to Constant FY 99 Dollars	8.53	8.53	8.53	8.53	8.53
Total Cost for Demilitarization	8.53	8.53	8.53	8.53	8.53
<i>Cost per Pound</i>	\$ 8.53	\$ 8.53	\$ 8.53	\$ 8.53	\$ 8.53
Resale of RDX**	\$ 6.53	\$ 6.53	\$ 6.53	\$ 6.53	\$ 6.53
Total (Cost) Profit per pound	\$ (2.00)	\$ (2.00)	\$ (2.00)	\$ (2.00)	\$ (2.00)

** Market Supports 50% of Baseline RDX Cost

The costs for demilitarizing TPE propellants are obtained from subject matter experts within the industry. The five scenarios presented are quantity variations of 100,000 pound increments, starting at 100,000 pounds. The labor and material costs for the demilitarization process of TPE propellants is presented in Table X. The totals for both labor and material costs include a 12% general and administrative (G&A) cost.

The labor costs are based on labor hours (i.e., hours per year) multiplied by a labor rate. The labor rate used here is \$65 per hour. Two full-time employees (FTE) are required for this process and have 1,776 effective hours per year per batch for this process. The materials used in the demilitarization process are methanol and liquid nitrogen. The cost for liquid nitrogen is not captured due to the insignificant amounts used in the process. Methanol costs per pound is \$32.28. As shown in Table 4, the total cost for demilitarization of TPE propellant ranges from \$34.87 to \$32.80, depending on the quantity. The baseline cost of RDX used for this cost and environmental analysis was \$13.06 per pound. It is assumed that the market for reclaimed RDX will support 50% of

the baseline virgin RDX cost. Thus, the resale of RDX results in \$6.53 per pound. The net total cost of the reclamation of RDX ranges from \$28.34 to \$26.27 per pound (Table X).

Table X Demilitarization Costs for TPE Propellant

Pounds of Energetic per Year		100,000	200,000	300,000	400,000	500,000
Direct Labor (\$/lb)	\$	2.59	\$ 1.29	\$ 0.86	\$ 0.65	\$ 0.52
Direct Material	\$	32.28	\$ 32.28	\$ 32.28	\$ 32.28	\$ 32.28
Subtotal Direct Production	\$	34.87	\$ 33.57	\$ 33.14	\$ 32.93	\$ 32.80
<i>Cost per Pound</i>		<i>\$ 34.87</i>	<i>\$ 33.57</i>	<i>\$ 33.14</i>	<i>\$ 32.93</i>	<i>\$ 32.80</i>
Resale of RDX**	\$	6.53	\$ 6.53	\$ 6.53	\$ 6.53	\$ 6.53
Total (Cost) Profit per pound	\$	(28.34)	\$ (27.04)	\$ (26.61)	\$ (26.40)	\$ (26.27)
** Market supports 50% of Baseline RDX Cost						

SYSTEMS INTEGRATION

Of course the goal would be to have the model-based approach completely automated with Internet user access. It was the general opinion of the workshop attendees that initial efforts should focus on applying the models in series to demonstrate the principle of identifying propellant candidates and obtaining environmental and demil const information. The attempt to generate specific computer code would be a separate effort in itself and should be delayed pending the completion of the initial development efforts.

SUMMARY AND CONCLUSION

1. Three SERDP Model-Based Formulations Workshops attended by experts in the field were conducted to review the status and to agree upon next steps needed to meet the objectives of this modeling approach. The proceedings of these workshops have been published. One of the workshops was held as a 1998 Joint Propulsion Meeting JANNAF Specialist Session.
2. A modeling architecture was developed which allows the estimation of propellant processing environmental, demilitarization, labor and materials costs based on user's environmental and weapons performance requirements. This architecture consists of a Performance Algorithm, a Resource Recovery Recycle and Reuse (R3) Demil Algorithm, and an automated process simulation. The environmental cost analysis results are obtained from the application of Environmental Cost Analysis Method (ECAMSM) to the propellant processing simulation. This achievement initially has focused upon gun propellant technology. This architecture can be readily expanded to include explosives, rocket propellants and pyrotechnics. It is conceivable this modeling effort can become the DoD and Industry Standard for the development of new energetic materials.

3. A performance algorithm was developed using existing thermodynamic and interior ballistics codes. For execution of the algorithm, a propellant formulation library, propellant burning rate database, and a propellant vulnerability predictor were established.
4. A Resource Recovery Recycle and Reuse Algorithm was developed. This algorithm estimates the cost for demilitization, recovery of key ingredients and treatment/disposal of waste. This algorithm stresses the implementation of new technology for resource recovery recycle and reuse.
5. A process simulation was developed which identifies the resource requirements and waste streams, the activities, time and cost associated with each activity, for both continuous and batch propellant processing. This simulation provides the basis for activities based costing and allows the calculation of environmental and nonenvironmental costs. This simulation has been automated using commercially available software, and has the built in flexibility to be adapted to any facility.
6. Modeling of environmental costs was achieved through the application Environmental Cost Analysis Methodology. ECAMSM historically has been used to perform economic analysis upon existing operational facilities. This is a unique application in that ECAMSM is applied to a process simulation.
7. Commercially available energy modeling software was identified which determines the energy consumption and the associated costs for processing propellant formulations. The energy model is flexible enough to provide information for different formulations and processing conditions and allows for the analysis of energy consumption at very specific levels. Outputs from this energy model can be readily used in the process simulation and resulting environmental cost analysis.
8. The overall architecture was successfully demonstrated. Inputs into the model included the muzzle velocity, maximum internal gun pressure and that the propellant be lead free. Environmental cost information such as cost for waste, air emissions, permitting, pollution prevention, documentation was determined for a 200-pound batch of propellant which meet the above environmental and performance requirements. With the output in the form of an output worksheet, the data can be represented with a variety of graphical options. Both a solventless and a solvent process propellant resulted as potential candidates that meet the input requirements. This demonstration shows how comparisons of the environmental costs of two different formulations that meet environmental and performance requirements can be made.
9. To date, this project has resulted in six technical reports, four invited presentations, one open literature publication, and two publications submitted for review in the open literature journal Clean Products and Processing.

NEXT STEPS

1. A critical next step is to demonstrate the ability to integrate the Performance and R3 Algorithm with the process simulation and demonstrate the remote execution of the model through a designated web site. The codes, databases and algorithms used in the model-based formulations approach will be integrated to be executed simultaneously in an automated fashion by the non-expert user.
2. The process simulation used to demonstrate the feasibility of the model-based approach does contain some general assumptions and estimations for time and cost. It is necessary to expand the simulation by providing more detail and specifics for certain process activities. Also, it is very important that this simulation be validated by comparing the predicted results with live process runs.
3. Automation of the performance simulation including all existing type-classified gun propellant formulations needs to be performed. This would require developing reasonable default values for properties of the formulations that might not be known (such as burning rate), but that are required for execution of the performance simulation.

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